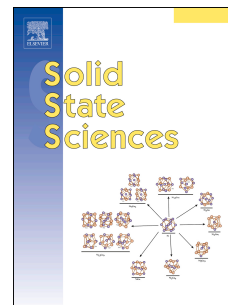


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Jean Etourneau, Samir F. Matar



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High Pressure in Solid State Chemistry: Combined Experimental and Modeling Approach for Assessing and Predicting Properties

Jean Etourneau. ICMCB-Université de Bordeaux- CNRS. 33600 Pessac. France

Email: jean.etourneau@icmcb.cnrs.fr

Samir F. Matar*. Lebanese German University (LGU). Sahel-Alma Campus, P. O. Box 206, Jounieh. Lebanon.

Email: s.matar@lgu.edu.lb (corresponding author)

**Formerly at CNRS-ICMCB-University of Bordeaux. France*

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Abstract.

The thermodynamic pressure parameter has been thoroughly used with mastery by Gérard Demazeau throughout his rich career in solid state chemistry and materials sciences and more recently in biosciences. After a review of such works, focus is made in this topical article on his contribution together with his team in the field of hard materials based on light elements B, C, N with a proposition of a new ultra-hard carbon nitride C_2N on one hand and on the structural transformations under high pressures of perovskite into postperovskite with a change of dimensionality from 3D to 2D and related oxides, regarding the arrangement of octahedra, on the other hand. Investigation and concepts first arising from experimental observables are shown to be aided and accelerated via first principles calculations of energy and energy-related quantities.

I-Introduction

In this article we wish to highlight some significant and original aspects of the scientific work of late Gérard Demazeau who has developed during many decades the high pressure technology in a large range of temperatures to make new materials through solid-solid, solid-oxygen and solvo-thermal chemical reactions [1, 2].

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